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4. NATIONAL LABS:

Molecular whiz tackles carbon capture, natural gas

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BERKELEY, Calif. -- When he started fiddling around in the laboratory, building metal ions into pieces of crystalline scaffolding that resemble tinker toys, Omar Yaghi had no higher purpose in mind.

Back then, his office was full of models. They depicted different metal-organic frameworks -- or MOFs -- made by mixing organic chemicals and metals such as zinc oxide in different proportions and conditions.

Yaghi and his research partners at Arizona State University were adding one or two more structures to their collection every day. They did little with their inventions except publish papers, and Yaghi was happy with that.

"I went into chemistry, really, for the beauty of molecules," he said. "I didn't want to solve any societal problem."

Omar Yaghi joined the Lawrence Berkeley National Laboratory last month as director of the lab's Molecular Foundry. Yaghi is known for designing structures called metal-organic frameworks (MOFs) that could capture carbon dioxide from power plants or expand the capacity of fuel tanks for natural gas-powered vehicles. Photo courtesy of the Lawrence Berkeley National Lab.

Yaghi hadn't realized that his structures, further refined over the next decade at the University of Michigan and the University of California, Los Angeles, might someday prove a crucial tool in mankind's mastery of natural gas.

Their promise for energy technologies such as natural gas vehicles, hydrogen fuel cells and carbon capture has helped catapult Yaghi to the top of his field and placed him on some observers' short lists for the Nobel Prize in chemistry. Last year, Thomson Reuters ranked him as the No. 2 chemistry researcher in the world.

Yaghi was born in 1965 in Amman, Jordan, and grew up as one of 13 children in a home surrounded by cows, grapevines and olive orchards. He left for the United States at age 15 to pursue his studies, and a few years later he started tinkering with molecules as a graduate student at the University of Illinois.

That went on for years as an academic exercise. In the late 1990s at Arizona State, when a mentor from the business world asked him what good his structures served, Yaghi was offended.

"I'm supposed to be addressing intellectual challenges," he recalls thinking. "I'm not supposed to be making the next fastest car or the next best fuel and all that stuff. I was supposed to do science for the sake of science."

But his structures' potential for fuel tanks forced him to rethink that opinion.

They could be especially useful if the United States wants to run more of its vehicles on natural gas. There are already about 112,000 natural gas vehicles on American roads and 13 million worldwide, but storing natural gas in vehicles is far more difficult than storing gasoline or diesel.

Yaghi's structures -- which resemble a fine white powder -- could double the amount of gas in a storage tank without requiring the fuel to be compressed under such intense pressure. German chemical giant BASF Corp., an early investor in Yaghi's research, is now commercializing the technology with hopes that it could become a mainstay in fuel tanks worldwide.

As the new director of Lawrence Berkeley National Laboratory's Molecular Foundry, Yaghi will oversee a research team that is looking for the answers to those sorts of big energy challenges at the molecular level.

But Yaghi, who has said that he would have been a gardener or a pianist if he hadn't gone into chemistry, will keep searching for beauty in basic science, too.

"That's what I really enjoy," he said during an interview in January, three weeks into his new job. "Every morning when I go to the foundry, I feel I'm very fortunate to be able to do the things that I really enjoy and still not lose out on helping solve societal problems."

Solving the density problem

Because the high thermal energy of gas molecules keeps them far apart from one another, liquefying or compressing the gas to overcome that low density takes energy -- so natural gas vehicles still tend to get fewer miles between trips to the pump compared to gasoline-fueled vehicles.

On top of that, liquefied and compressed natural gas tanks must be built to exacting specifications to withstand the pressure inside the tank, making the vehicles harder to design.

That is where MOFs would come in.

If the gas molecules were bees, Yaghi said, a well-designed MOF would be a honeycomb, its porous openings giving the gas molecules more places to stay than they would have with a solid surface. According to BASF, the German chemical firm, a single gram of MOFs has a surface area of 1,100 to 2,100 square meters, the equivalent of several football fields.

The materials that make up MOFs are relatively common and cost $7 to $15 per pound, Yaghi said, though the chemical process used to make them is more exacting and costly.

An automaker using MOFs would buy them and add them to the fuel tank, giving it more capacity or allowing the internal pressure to be ratcheted down without reducing the vehicle's range. The substance could be recovered and reused when a vehicle reaches the end of its useful life.

Scientists have probably already come up with MOFs that are good enough to do that job, according to Randall Snurr, a chemical engineering professor at Northwestern University who also designs and tests the structures.

His team, like other research groups in the field, claims to have found MOFs that would meet a U.S. Department of Energy target of designing a fuel tank that can hold the same amount of methane as a compressed natural gas (CNG) tank at less than one-fifth the pressure. Companies that hope to use the technology must now deal with practical questions such as the cost and durability of their structures, and figure out how well they would stand up to the impurities in natural gas.

Those questions will be key if Americans want to use natural gas -- now at historically low prices -- as a replacement for oil.

"Gasoline's a really good fuel," Snurr said. "It has really high energy density, and I think with natural gas the dream would be to do as good as gasoline."

Next in line

Scientists were already experimenting with MOFs and a similar set of structures called zeolites when Yaghi started his work.

The new director of the Molecular Foundry gained a reputation as a leader in the field when he "came up with one of the first materials that really worked," Snurr said.

Many of the early structures designed by other researchers were beautiful, Snurr said, but they would break down when they were removed from the solvent in which they were formed. Yaghi caught people's attention by coming up with a chemical process that made the same building blocks into porous but stable materials.

Perhaps more important, Yaghi coined the term "MOF" and popularized it. Yaghi has designed other structures, which he dubbed ZIFs, COFs and CATs, but those have yet to become as well-known.

"It's helped the field a lot," Snurr said of the MOF moniker. "People just like the term. It's self-explanatory and it's simple."

Sometimes, a snappy name matters.

Just ask Berkeley Lab director Paul Alivisatos, who helped brainstorm the name of the six-year-old Molecular Foundry and became its first director. He is himself a nanotechnology expert and checks in three spots behind Yaghi on the Thomson Reuters list of the most-cited chemistry researchers.

Alivisatos said he wanted the new lab to have an image as a place where people could tinker with the building blocks of the elements, similar to the forges where people in past ages learned to work with iron, bronze and steel.

Plus, there were too many other research centers with the word "nano" in their names, he said during an interview at his office in the hills above the University of California.

Alivisatos has designed tiny structures of his own, such as a class of nanocrystals called "quantum dots" that may help solar panels more efficiently convert light into electricity. After leading the foundry and Berkeley Lab's materials division, he succeeded Energy Secretary Steven Chu as head of the entire laboratory when President Obama appointed Chu to the Cabinet.

Researchers from around the world can apply for time to work with the foundry's specialized equipment at its office in the hills above the University of California's Berkeley campus. It received just under 300 applications in 2010, more than the facility received in its first several years combined.

'Totally different' way to capture carbon

Years down the line, MOFs could also find use in hydrogen fuel cells, which hold promise as an emissions-free transportation fuel but remain too expensive for the marketplace. Favored by the George W. Bush administration, hydrogen has lost some of its funding as the Obama administration has focused more heavily on battery research and other improvements key to electric cars.

Still, DOE announced last month it will give Berkeley Lab $2.1 million over three years to study the use of MOFs for that purpose. General Motors Co. and the National Institute of Standards and Technology will also fund the research.

The molecules that Yaghi pioneered could also theoretically help power plants stash carbon dioxide underground without losing as much energy when they capture it.

Most pilot projects to date have used amine-based chemical absorbents to capture the carbon from flue gas after a fuel such as coal is burned. Bringing that technology to scale requires massive stacks to make sure the amine comes into contact with the CO_2, and because separating the captured carbon from the amine solution takes a great deal of heat, the equipment could consume more than a quarter of the energy in the fuel being burned.

Exposing carbon dioxide to a MOF may allow the carbon to be captured in a smaller space, and could also let it be separated into a pure stream without siphoning off as much of a power plant's main product -- electricity.

Yaghi published some of his research on that topic in 2009, wowing his colleagues in the field. "The genius of the materials that Professor Yaghi has developed is their enormous capacity for CO_2," said Joseph Hupp, a Northwestern University chemist who has learned to make MOFs that separate carbon emissions from methane (***Greenwire***, June 30, 2009).

Experts imagine a MOF-loaded capture system with two stacks.

The flue gas would start by traveling into the first stack, where the MOFs would capture the carbon dioxide. The rest of the gas -- mainly water vapor and nitrogen -- would be released into the atmosphere.

Then, the first stack would be closed and the MOFs would be heated up to break their weak bonds with carbon dioxide. Meanwhile, the process would be repeating itself in the second stack. At any given time, one of the two stacks would be capturing carbon and the other would be releasing it from the MOFs into a pure stream, ready for storage underground or for some other use.

Energy Secretary Steven Chu, the former director of Berkeley Lab, mentioned that idea during a hearing last week, when Sen. Rob Portman (R-Ohio) asked him how the agency's work will help deploy carbon capture into the marketplace.

At the moment, the best-known carbon capture technologies would increase the price of electricity enough that it "would not spur China or India into using these technologies," Chu said. Because the small sandy particles have such a large surface area, a stream of carbon dioxide could be treated in a smaller space, shrinking the needed equipment and saving on construction costs.

"We're investing a lot of resources to decrease the size of these capture stacks," Chu told the Senate Energy and Natural Resources Committee. "It's a totally different way of doing it."

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